

Modeling of Nanoscale Multiphase Transport Phenomena and Its Application to Head-Disk Interface of Hard Disk Drive System

Abstract

We will present the fundamental scientific tools, as well as construct cohesive schemes for the multiphase transport phenomena in the nanoscale confined systems including ultra thin liquid film, airbearing, and multilayer solid films.

Our talk here focuses on the understanding of the dynamic behavior of molecularly thin polymeric liquid films, relevant to the emerging field of nanotechnology, especially for simulating the nanoscale transport processes to achieve durability and reliability in nanoscale devices. The unified and hybrid description of perfluoropolyether (PFPE) lubricants including mesoscopic interpretation, microscopic simulation, and molecular design tools will be given. A method for extracting spreading properties from the scanning microellipsometry and the rheological characterization of PFPEs are examined. Mesoscopic theories, including the thermodynamics of evaporation, stability analysis, mesoscale mass transfer, and capillary waves are introduced to describe thin PFPE film dynamics. The on-lattice simple reactive sphere model for qualitatively examining the fundamentals of PFPE dynamics is illustrated. An off-lattice, coarse-grained, bead-spring Monte Carlo technique is also introduced to capture a detailed internal structure of PFPE molecules, and the molecular dynamics simulation with the Langevin equation is implemented for a full-scale dynamic structural analysis of PFPE thin films. By systematically tuning the endgroup strengths of PFPE, we examined the physicochemical properties of nanostructural lubricant films for various PFPE/solid surface pairings. Our tools accurately describe the static and dynamic behaviors of PFPE films which are consistent with experimental findings and provide a suitable starting point for describing the fundamental mechanisms of film dewetting and rupture due to instability arising from temperature and pressure inhomogeneities. The next generation head-disk interface design in information storage devices is used to examine the couplings of thin liquid lubricant film with high Knudsen number (Kn) airbearing and heat conduction in nanoscale solids. Modified Reynolds equations based on the Boltzmann transport equation will be introduced to examine nanoscale fluid mechanics airbearing simulation, and heat conduction in solids especially for high Kn using lattice Boltzmann method.